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Data Mining and Machine Learning
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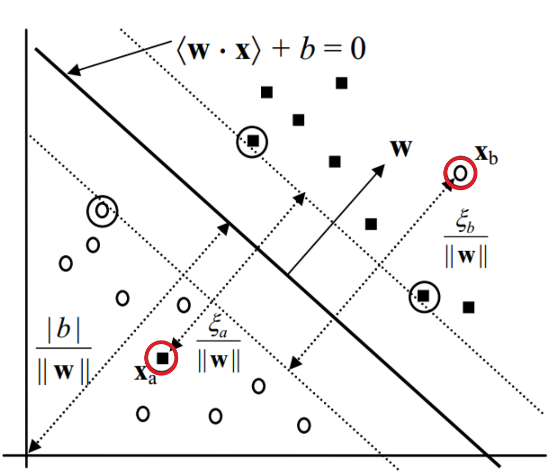
Soft margin optimization

Minimize $\dfrac{||w||}{2} + \sum_{i=1}^{N} \xi_i^2$

Subject to

$$\begin{aligned} &\xi_i \geq 0 \\ &\langle w \cdot x \rangle + b > 1 - \xi_i, \quad \text{if } y_i = 1 \\ &\langle w \cdot x \rangle + b < -1 + \xi_i, \quad \text{if } y_i = -1 \end{aligned}$$

- Constraints include requirement that error terms are non-negative
- Again the objective function is quadratic

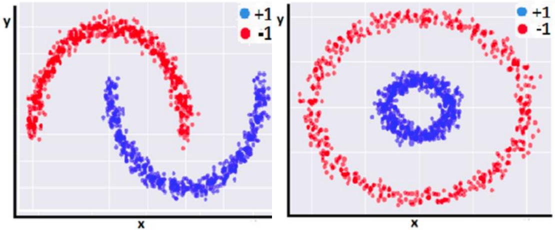


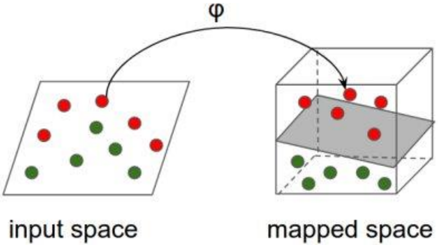
The non-linear case

- How do we deal with datasets where the separator is a complex shape?

- Geometrically transform the data
  - Typically, add dimensions

- For instance, if we can "lift" one class, we can find a planar separator between levels



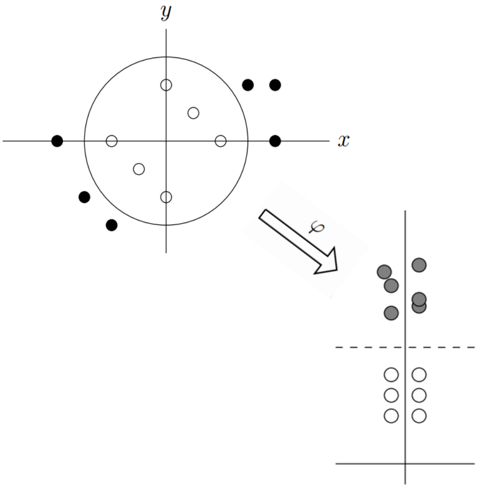


Geometric tranformation

- Consider two sets of points separated by a circle of radius 1
- Equation of circle is $x^2 + y^2 = 1$
- Points inside the circle $x^2 + y^2 < 1$
- Points outside circle $x^2 + y^2 > 1$
- Transformation

$$\varphi : (x, y) \mapsto (x, y, x^2 + y^2)$$

- Points inside circle lie below z = 1
- Point outside circle lifted above z = 1



SVM after transformation

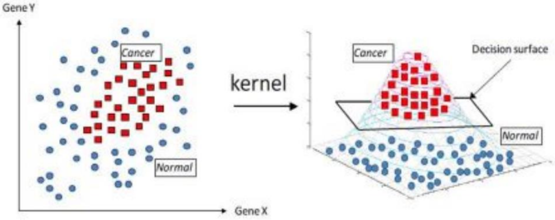
- SVM in original space

$$\operatorname{sign}\left[\sum_{i \in sv} y_i \alpha_i \langle x_i \cdot z \rangle + b\right]$$

- After transformation

$$\operatorname{sign}\left[\sum_{i \in sv'} y_i \alpha_i \langle \varphi(x_i) \cdot \varphi(z) \rangle + b\right]$$

- All we need to know is how to compute dot products in transformed space



Dot products

- Consider the transformation

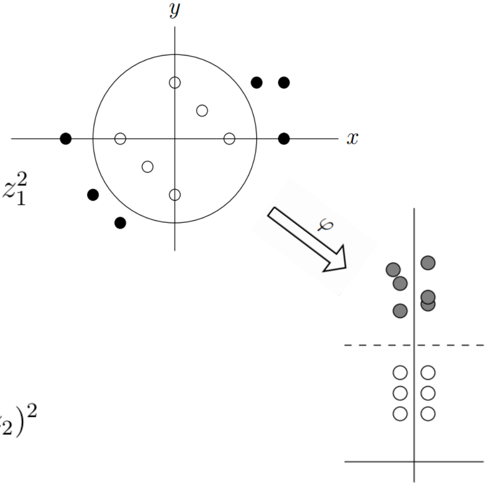
$$\varphi : (x_1, x_2) \mapsto (1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, \sqrt{2}x_1x_2, x_2^2)$$

- Dot product in transformed space

$$\begin{aligned}\langle \varphi(x) \cdot \varphi(z) \rangle &= 1 + 2x_1z_1 + 2x_2z_2 + x_1^2z_1^2 \\ &\quad + 2x_1x_2z_1z_2 + x_2^2z_2^2 \\ &= (1 + x_1z_1 + x_2z_2)^2\end{aligned}$$

- Transformed dot product can be expressed in terms of original inputs

$$\langle \varphi(x) \cdot \varphi(z) \rangle = K(x, z) = (1 + x_1z_1 + x_2z_2)^2$$



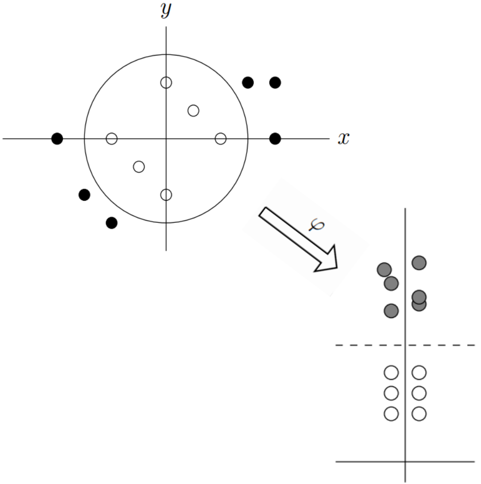
Kernels

- K is a *kernel* for transformation φ if

$$K(x,z) = \langle \varphi(x) \cdot \varphi(z) \rangle$$

- If we have a kernel, we don't need to explicitly compute transformed points
- All dot products can be computed implicitly using the kernel on original data points

$$\text{sign}\left[\sum_{i \in sv'} y_i \alpha_i \langle \varphi(x_i) \cdot \varphi(z) \rangle + b\right]$$



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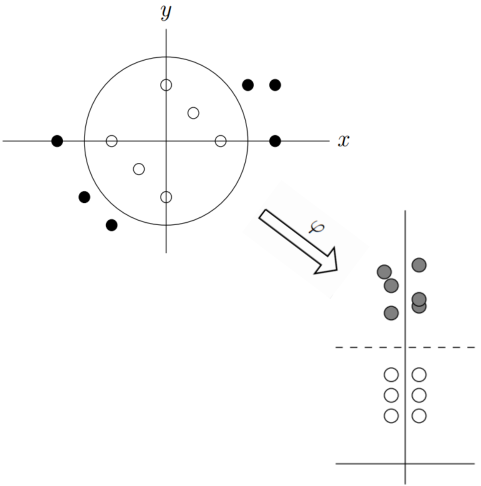
$$K(x, z) = \langle \varphi(x) \cdot \varphi(z) \rangle$$

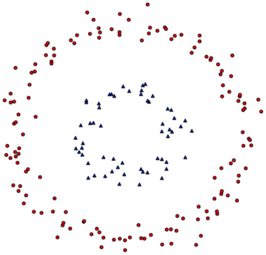
- If we have a kernel, we don't need to explicitly compute transformed points
- All dot products can be computed implicitly using the kernel on original data points

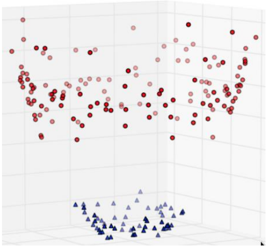
$$\text{sign}\left[\sum_{i \in sv'} y_i \alpha_i K(x_i, z) + b\right]$$



Kernels

- If we know K is a kernel for some transformation φ, we can blindly use K without even knowing what φ looks like!
- When is a function a valid kernel?
- Has been studied in mathematics – Mercer's Theorem
    - Criteria are non-constructive
- Can define sufficient conditions from linear algebra



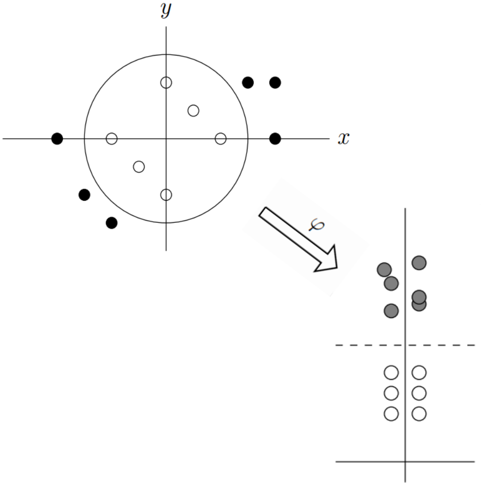


Kernels

- Kernel over training data $x_1, x_2, \ldots, x_N$ can be represented as a *gram matrix*

$$K = \begin{array}{c c} & \begin{array}{cccc} x_1 & x_2 & \cdots & x_N \end{array} \\ \begin{array}{c} x_1 \\ x_2 \\ \vdots \\ x_n \end{array} & \left[\begin{array}{cccc} & & & \\ & & & \\ & & & \\ & & & \end{array} \right] \end{array}$$

- Entries are values $K(x_i, x_j)$
- Gram matrix should be *positive semi-definite* for all $x_1, x_2, \ldots, x_N$



Known kernels

- Fortunately, there are many known kernels
- Polynomial kernels

$$K(x,z) = (1 + \langle x \cdot z \rangle)^k$$

- Any K(x,z) representing a similarity measure
- Gaussian radial basis function – similarity based on inverse exponential distance

$$K(x,z) = e^{-c|x-z|^2}$$